

Coulomb energy of axially deformed nucleus

Ning Wang,¹ Xuexin Yu,¹ and Min Liu^{*1,2}

¹*Department of Physics, Guangxi Normal University, Guilin 541004, P. R. China*

²*College of Nuclear Science and Technology,
Beijing Normal University, Beijing, 100875, P. R. China*

Abstract

We previously proposed a formula for calculating the Coulomb energy of spherical nucleus with Wood-Saxon charge distribution. In this work, the analytical formula is extended for description of the Coulomb energy of nucleus with β_2 deformation.

* Corresponding author : lium_816@hotmail.com

The calculation of the Coulomb energy for complicated charged system with small computing effort and high accuracy is a great challenge in physics and quantum chemistry research [1–3]. For a system with an arbitrary charge distribution $\rho(\mathbf{r})$, the direct term of the Coulomb energy can be calculated with

$$E_C = \frac{e^2}{2} \iint \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}d\mathbf{r}'. \quad (1)$$

However, the six-dimensional integration in Eq.(1) is very time-consuming and becomes a bottleneck in the large-scale calculations of potential energy surfaces of nuclear systems. In this work, we attempt to propose an analytic expression for calculating the Coulomb energy of nucleus with both the nuclear surface diffuseness and nuclear β_2 deformation being taken into account. For reader's convenience, the approach to calculate the Coulomb energy of a nuclear system proposed in our previous work [1] is reviewed firstly, and then the analytical formula for calculating the Coulomb energy of spherical nucleus with Woods-Saxon density distribution will be extended for description of the Coulomb energy of nucleus with β_2 deformation.

The Coulomb energy of an arbitrary nuclear system can be obtained by

$$E_C = \frac{e}{2} \int \rho(\mathbf{r}) V_C(\mathbf{r}) d\mathbf{r}, \quad (2)$$

where $V_C(\mathbf{r})$ is the Coulomb potential which is obtained by solving the Poisson equation

$$\nabla^2 V_C(\mathbf{r}) = -4\pi e \rho(\mathbf{r}). \quad (3)$$

The charge distribution of a nucleus is usually described by a Woods-Saxon form,

$$\rho(r) = \frac{\rho_0}{1 + \exp(\frac{r-\mathcal{R}}{a})}. \quad (4)$$

Where, ρ_0 and a denote the central charge density and the surface diffuseness, respectively. \mathcal{R} defines the distance from the origin of the coordinate system to the point on the nuclear surface. For an axially deformed system, \mathcal{R} is expressed as,

$$\mathcal{R}(\theta) = R_0 [1 + \beta_2 Y_{20}(\theta) + \dots]. \quad (5)$$

In the calculation of Coulomb energy of nucleus as a function of nuclear deformation, we remain the central charge density ρ_0 of the nucleus unchanged by using the conservation of

charge number and varying the half-density radius R_0 to consider the effect of incompressibility of nuclear matter in the nucleus.

The Poisson equation is solved by a code **hwscyl** (a Fortran subroutine in FISHPACK [4]) which is an adaptive fast solver for solving a five-point finite difference approximation to the modified Helmholtz equation in cylindrical coordinates using a centered finite difference grid. We calculate the Coulomb potential in cylindrical coordinates within a region $x = 0 \sim 40$ fm and $z = -40 \sim 40$ fm (using a grid with step size 0.1 fm). It is known that when $r \gg \mathcal{R}$, the asymptotic behavior of the Coulomb potential of a nucleus is $V_C = eZ/r$, which gives the boundary condition in solving the Poisson equation. The Coulomb energy of an arbitrary axially deformed nuclear system can be obtained with a two-dimensional integration over the Coulomb potential $V_C(\mathbf{r})$ which can be calculated with the very fast solver for the Poisson equation mentioned above.

In our previous work [1], we investigated the Coulomb energies of spherical nuclei with Wood-Saxon charge distributions. The central charge density of a nucleus is obtained with the Skyrme energy density functional together with the extended Thomas-Fermi (ETF) approach [5]. The nuclear surface diffuseness a varies from 0.1 to 1.2 fm in which the central charge density is remained unchanged. We find that the Coulomb energies of spherical nuclei with Woods-Saxon charge distributions can be well described with an analytical expression based on the leptodermous expansion [6],

$$E_{\text{Coul}} = E_C^{(0)} F(\omega) \quad (6)$$

with [1]

$$F(\omega) = 1 - \frac{5}{2}\omega^2 + c_3\omega^3 + \omega^4 + c_5\omega^5 + c_6\omega^6 + \dots \quad (7)$$

Where, $\omega = \frac{\pi}{\sqrt{3}} \frac{a}{R}$ and $E_C^{(0)}$ denotes the Coulomb energy of a spherical nucleus with uniform charge distribution,

$$E_C^{(0)} = \frac{3}{5} \frac{Z^2 e^2}{R}. \quad (8)$$

Z denotes the charge number of the nucleus and $R = [Z/(\frac{4\pi}{3}\rho_0)]^{1/3}$ is the corresponding radius of a spherical nucleus with uniform charge distribution. By fitting the calculated Coulomb energies with numerical integrations for a number of spherical nuclei along the β -stability line, we obtained the coefficients $c_3 = 3.005$, $c_5 = -4.822$, $c_6 = 2.934$.

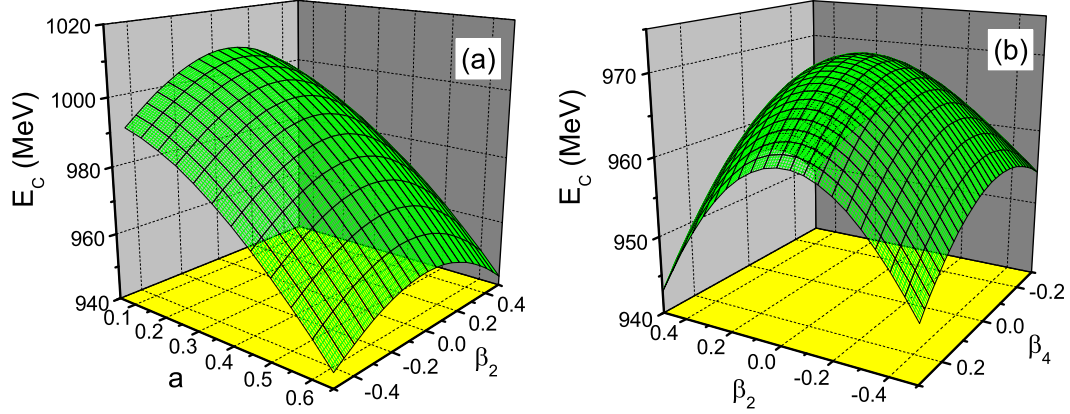


FIG. 1: (Color online) Coulomb energies of ^{238}U as a function of nuclear surface diffuseness a and quadrupole deformation β_2 (a); and as a function of β_2 and β_4 (b).

With the same approach, we investigate the Coulomb energies of deformed nuclei. In Fig.1 (a), we show the calculated Coulomb energy of ^{238}U as a function of nuclear surface diffuseness a and quadrupole deformation β_2 , and we show the corresponding Coulomb energy as a function of β_2 and β_4 (with $a = 0.55$ fm) in Fig.1(b). One can see that the Coulomb energy decreases with increase of the nuclear surface diffuseness and of the deformation. In this work, we write the Coulomb energy of a nucleus as

$$E_{\text{Coul}} = E_C^{(0)} F(\omega) G(\omega, \beta), \quad (9)$$

with a factor $G(\omega, \beta)$ to consider the influence of nuclear deformation. For nucleus with β_2 deformation, we assume that the factor $G(\omega, \beta)$ has a form

$$G(\omega, \beta_2) = 1 - \frac{1}{4\pi} \beta_2^2 + b_1 \omega \beta_2^2 + b_2 \omega^2 \beta_2^2 + b_3 \beta_2^3 + b_4 \beta_2^4 + \dots \quad (10)$$

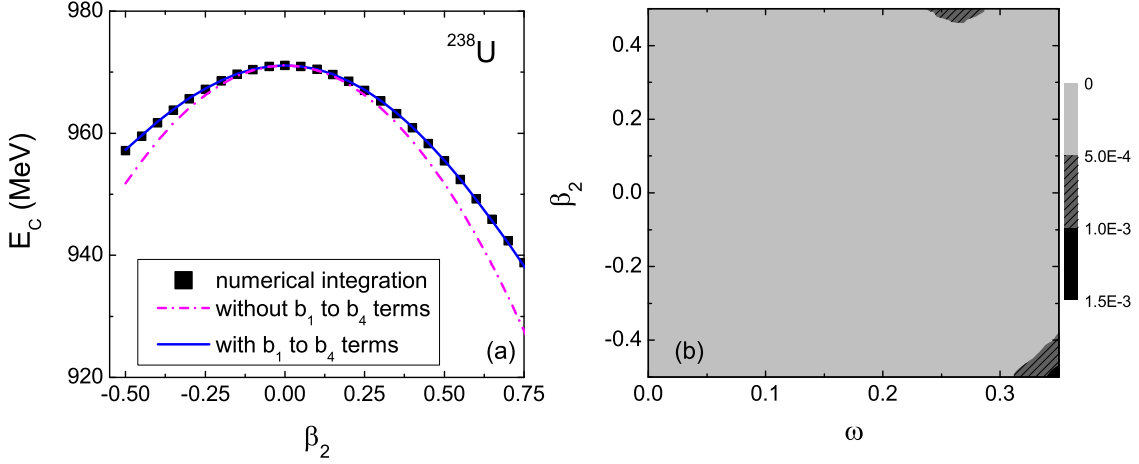


FIG. 2: (Color online) (a) Coulomb energy of ^{238}U as a function of β_2 deformation (with $a = 0.55$ fm). The squares denote the results with numerical integration [with Eq.(2)]. The dot-dashed curve and the solid curve denote the results of Eq.(9) without and with the b_1 to b_4 terms being taken into account, respectively. (b) Relative deviations $|E_{\text{Coul}} - E_C|/E_C$ of the Coulomb energies from the numerical integration results. E_{Coul} denotes the calculated Coulomb energy with Eq.(9) and (10). The region with light gray denote that the relative deviations are smaller than 0.05%.

TABLE I: Values of $\omega = \frac{\pi a}{\sqrt{3}R}$ for some nuclei by taking $a = 0.55$ fm and $R = 1.2A^{1/3}$ fm.

	^{16}O	^{40}Ca	^{90}Zr	^{144}Sm	^{208}Pb	^{238}U	$^{298}114$
ω	0.33	0.24	0.19	0.16	0.14	0.13	0.12

Where the term $-\frac{1}{4\pi}\beta_2^2$ is presented by Greiner and Maruhn in Ref. [7]. By fitting the calculated Coulomb energies with Eq.(2) as a function of surface diffuseness ($a \leq 0.7$ fm) and quadrupole deformation ($|\beta_2| \leq 0.5$) for a number of nuclei along the β -stability line, we obtain the coefficients $b_1 = \frac{1}{4\pi}$, $b_2 = 0.188$, $b_3 = -0.007$ and $b_4 = 0.018$.

In Fig.2(a), we show the Coulomb energy of ^{238}U as a function of nuclear quadrupole deformation β_2 . The squares denote the results with Eq.(2). The dot-dashed curve and the solid curve denote the results of Eq.(9) without and with the b_1 to b_4 terms being taken into account, respectively. One can see that the higher-order terms of deformation are still

required for system with large deformation. In Fig.2(b), we show the relative deviations $|E_{\text{Coul}} - E_C|/E_C$ of the Coulomb energies from the numerical results for a number of nuclei $A = 16 \sim 300$ varying the surface diffuseness ($a \leq 0.7$ fm) and the quadrupole deformation ($|\beta_2| \leq 0.5$). E_{Coul} denotes the calculated Coulomb energy with Eq.(9) and (10). From Fig.2, one can see that the Coulomb energy obtained with the analytical formula Eq.(9) is close to the calculated results with numerical integration for most cases. In Table 1, we list some typical ω values of a series of nuclei from light to heavy. For intermediate and heavy nuclei, ω has a value about $0.1 \sim 0.25$, the corresponding relative deviations of the Coulomb energies with Eq.(9) are smaller than 0.05% [denoted by light gray in Fig.2(b)] for almost all cases with $a \leq 0.7$ fm and $|\beta_2| \leq 0.5$. For light nuclei, the corresponding values of ω are larger than 0.25 in general and the relative deviations of the Coulomb energies with Eq.(9) slightly increase for some cases with strong deformations. It is known that the charge distributions of light nuclei are usually described by gaussian functions rather than the Woods-Saxon form. The analytical expression of the Coulomb energy of a system with gaussian charge distribution can be found in Refs. [1, 6].

In summary, the Coulomb energy of axially deformed nucleus with Wood-Saxon charge distribution has been investigated. The Coulomb energy of a nuclear system was numerically calculated with a two-dimensional integration over the Coulomb potential which was obtained by solving the Poisson equation. By fitting the numerically calculated Coulomb energies for a number of nuclei from $A = 16$ to 300 with β_2 deformed Wood-Saxon charge distribution, an analytical formula, that is a function of nuclear β_2 deformation and surface diffuseness, is finally obtained. The relative deviation of the Coulomb energy with the proposed formula is generally smaller than 0.05% for intermediate and heavy nuclei at normal deformations. For nuclear system with $|\beta_2| > 0.5$, such as fissioning system, the proposed formula could not be applicable, and the two-dimensional numerical integration over the Coulomb potential has to be performed to obtain accurate results.

ACKNOWLEDGEMENTS

This work is supported by National Natural Science Foundation of China, Nos 10875031, 10847004. The code to calculate the Coulomb energy of axially deformed system with

numerical integrations over the Coulomb potential is available from <http://www.imqmd.com>

- [1] Xuexin Yu, Min Liu and Ning Wang, *Mod. Phys. Lett. A* **25** (2010) 1275.
- [2] W. D. Myers and W. J. Świątecki, *Phys. Rev. C* **58** (1998) 3368.
- [3] F. R. Manby and P. J. Knowles, *Phys. Rev. Lett.* **87** (2001) 163001.
- [4] P. Swarztrauber, R. Sweet, *Efficient FORTRAN Subprograms for the Solution of Elliptic Equations*, NCAR Technical Report TN/IA-109, National Center for Atmospheric Research (1975) p.138.
- [5] Min Liu, Ning Wang, Zhuxia Li, Xizhen Wu and Enguang Zhao, *Nucl. Phys. A* **768** (2006) 80.
- [6] R. W. Hasse and W. D. Myers, *Geometrical Relationships of Macroscopic Nuclear Physics*, Springer-Verlag, Heidelberg (1988).
- [7] W. Greiner and J. A. Maruhn, *Nuclear Models*, Springer-Verlag Berlin Heidelberg, 1996, p.120.